Stabilizing Zr and Ti Cations by Interaction With a Ferrocenyl Fragment

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Published in:
Journal of the American Chemical Society

DOI:
10.1021/ja9077446

Publication date:
2009

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C15 C 0.29067(10) 0.24770(10) 0.40475(10) 0.0300(3) Uani 1 1 d . . .
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C12 C 0.28277(10) 0.21711(10) 0.54334(10) 0.0319(3) Uani 1 1 d . . .
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C1 C 0.18687(13) 0.42024(10) 0.35060(9) 0.0322(3) Uani 1 1 d . . .
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C16 C 0.03060(10) 0.28812(11) 0.47732(9) 0.0294(3) Uani 1 1 d . . .
C18 C 0.03438(11) 0.14504(10) 0.49532(11) 0.0336(3) Uani 1 1 d . . .
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C9 C 0.13652(14) 0.49426(11) 0.62127(11) 0.0386(4) Uani 1 1 d . . .
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C20 C 0.03339(11) 0.25010(11) 0.39733(10) 0.0324(3) Uani 1 1 d . . .
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C3 C 0.23595(13) 0.52692(10) 0.43610(11) 0.0352(3) Uani 1 1 d . . .
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C7 C 0.25857(12) 0.39396(12) 0.64468(9) 0.0357(3) Uani 1 1 d . . .
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C4 C 0.12904(13) 0.52810(10) 0.43006(12) 0.0376(3) Uani 1 1 d . . .
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C6 C 0.16299(13) 0.35578(11) 0.65434(8) 0.0332(3) Uani 1 1 d . . .
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C8 C 0.24269(15) 0.47946(12) 0.62408(11) 0.0392(4) Uani 1 1 d . . .
H8A H 0.2954 0.5229 0.6213 0.047 Uiso 1 1 calc R . .
C14 C 0.28290(12) 0.15920(11) 0.41355(12) 0.0379(4) Uani 1 1 d . . .
H14A H 0.2803 0.1181 0.3686 0.045 Uiso 1 1 calc R . .
F26 F 0.18729(7) 0.70883(5) 0.49761(5) 0.03399(18) Uani 1 1 d . . .
F32 F 0.04392(7) 0.74498(5) 0.75992(5) 0.02758(16) Uani 1 1 d . . .
C31 C 0.00246(9) 0.72657(8) 0.61861(7) 0.01869(19) Uani 1 1 d . . .
F46 F 0.20551(7) 0.68352(5) 0.66633(6) 0.02883(17) Uani 1 1 d . . .
C21 C 0.07692(9) 0.82641(7) 0.49393(7) 0.01996(19) Uani 1 1 d . . .
F22 F -0.03174(8) 0.94469(6) 0.46965(6) 0.0359(2) Uani 1 1 d . . .
C41 C 0.17319(10) 0.82809(7) 0.63337(6) 0.01879(18) Uani 1 1 d . . .
F42 F 0.17081(7) 0.97410(5) 0.59915(6) 0.03094(17) Uani 1 1 d . . .
F33 F -0.06155(9) 0.61123(7) 0.80788(5) 0.0420(2) Uani 1 1 d . . .
F35 F -0.16266(9) 0.56063(6) 0.53488(6) 0.0445(3) Uani 1 1 d . . .
F36 F -0.05754(8) 0.69289(6) 0.48415(5) 0.0348(2) Uani 1 1 d . . .
C42 C 0.21983(10) 0.90678(8) 0.63124(8) 0.0224(2) Uani 1 1 d . . .
C25 C 0.16959(12) 0.77619(9) 0.37162(8) 0.0290(2) Uani 1 1 d . . .
C32 C -0.00484(10) 0.70064(8) 0.70032(7) 0.0221(2) Uani 1 1 d . . .
C45 C 0.33646(10) 0.77770(9) 0.68694(7) 0.0250(2) Uani 1 1 d . . .
C35 C -0.11093(11) 0.60674(9) 0.59017(8) 0.0275(2) Uani 1 1 d . . .
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C34 C -0.11434(12) 0.58432(9) 0.67202(9) 0.0284(3) Uani 1 1 d . . .
C44 C 0.37753(10) 0.85773(11) 0.68479(8) 0.0285(3) Uani 1 1 d . . .
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C36 C -0.05374(10) 0.67617(8) 0.56551(7) 0.0230(2) Uani 1 1 d . . .
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B1 B 0.05714(10) 0.81754(8) 0.59464(8) 0.0189(2) Uani 1 1 d . . .
F43 F 0.35722(8) 1.00115(6) 0.65104(7) 0.0426(2) Uani 1 1 d . . .
C26 C 0.14397(10) 0.77221(8) 0.45434(8) 0.0243(2) Uani 1 1 d . . .
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C101 C -0.01939(11) 0.88777(9) 0.63407(8) 0.0258(2) Uani 1 1 d . . .
C23 C 0.06105(12) 0.89515(10) 0.35898(8) 0.0313(3) Uani 1 1 d . . .
F24 F 0.14957(11) 0.84316(8) 0.24323(6) 0.0526(3) Uani 1 1 d . . .
F23 F 0.01764(11) 0.95559(8) 0.31286(6) 0.0500(3) Uani 1 1 d . . .
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H102 H -0.0022(15) 0.9436(13) 0.6223(12) 0.031(5) Uiso 1 1 d . . .
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C10 0.0307(7) 0.0504(10) 0.0273(7) -0.0097(6) 0.0087(5) 0.0013(6)
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C22 0.0284(6) 0.0238(6) 0.0210(5) 0.0030(4) -0.0025(4) -0.0009(4)
F44 0.0233(4) 0.0641(7) 0.0366(5) 0.0038(5) -0.0058(3) -0.0123(4)
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F43 0.0413(5) 0.0349(5) 0.0515(6) -0.0035(4) -0.0037(4) -0.0205(4)
C26 0.0315(6) 0.0228(5) 0.0185(5) -0.0019(4) -0.0012(4) 0.0007(4)
C33 0.0367(7) 0.0244(6) 0.0175(5) 0.0008(4) 0.0010(4) -0.0076(5)
C101 0.0275(6) 0.0243(6) 0.0256(6) -0.0002(5) 0.0031(4) 0.0036(5)
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F24 0.0853(9) 0.0554(7) 0.0171(4) 0.0043(4) 0.0112(5) -0.0038(6)
F23 0.0757(8) 0.0463(6) 0.0280(5) 0.0174(4) -0.0054(5) 0.0090(6)
C24 0.0459(8) 0.0368(7) 0.0163(5) 0.0012(5) 0.0025(5) -0.0090(6)

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 are estimated using the full covariance matrix.  The cell esds are taken
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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F14 F 0.5303(2) 0.84688(16) 0.77876(13) 0.0395(7) Uani 1 1 d . . .
F15 F 0.3443(3) 0.89308(18) 0.75500(15) 0.0484(8) Uani 1 1 d . . .
C1 C 0.8153(4) 0.9196(3) 1.1519(2) 0.0287(11) Uani 1 1 d . . .
C2 C 0.8126(4) 0.8380(3) 1.1263(2) 0.0282(11) Uani 1 1 d . . .
C3 C 0.7583(4) 0.8166(3) 1.0586(2) 0.0264(11) Uani 1 1 d . . .
C4 C 0.7033(3) 0.8728(3) 1.0123(2) 0.0245(10) Uani 1 1 d . . .
C5 C 0.5637(3) 0.7104(3) 0.9671(2) 0.0283(10) Uani 1 1 d . . .
C6 C 0.6284(4) 0.7515(2) 0.9157(2) 0.0230(10) Uani 1 1 d . . .
C7 C 0.6675(4) 0.6987(3) 0.8569(3) 0.0277(11) Uani 1 1 d . . .
C8 C 0.6431(4) 0.6150(3) 0.8493(3) 0.0344(12) Uani 1 1 d . . .
C9 C 0.5773(4) 0.5799(3) 0.9019(3) 0.0348(12) Uani 1 1 d . . .
C10 C 0.3322(4) 0.9420(3) 0.8887(3) 0.0346(12) Uani 1 1 d . . .
C11 C 0.3756(4) 0.9524(3) 0.9626(3) 0.0334(12) Uani 1 1 d . . .
C12 C 0.4735(4) 0.9269(3) 0.9737(2) 0.0274(11) Uani 1 1 d . . .
C13 C 0.5335(3) 0.8921(2) 0.9152(2) 0.0233(10) Uani 1 1 d . . .
C14 C 0.5374(4) 0.6273(3) 0.9627(3) 0.0323(11) Uani 1 1 d . . .
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C15 C 0.7217(4) 0.8953(3) 0.8577(3) 0.0364(13) Uani 1 1 d . . .
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H15B H 0.7212 0.9563 0.8643 0.055 Uiso 1 1 calc R . .
H15C H 0.6986 0.8809 0.8035 0.055 Uiso 1 1 calc R . .
C16 C 0.7624(4) 0.9779(3) 1.1088(2) 0.0263(11) Uani 1 1 d . . .
C17 C 0.7112(3) 0.9542(3) 1.0414(2) 0.0239(10) Uani 1 1 d . . .
C18 C 0.4835(4) 0.8845(2) 0.8418(2) 0.0253(11) Uani 1 1 d . . .
C19 C 0.3881(4) 0.9075(3) 0.8277(3) 0.0343(12) Uani 1 1 d . . .
C20 C 0.5821(5) 0.6842(3) 0.2269(3) 0.0426(14) Uani 1 1 d . . .
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C22 C 0.4307(4) 0.6478(3) 0.2739(3) 0.0329(13) Uani 1 1 d . . .
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C23 C 0.5017(4) 0.6244(3) 0.3325(2) 0.0345(11) Uani 1 1 d . . .
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C26 C 0.5588(4) 0.8821(3) 0.2204(3) 0.0367(14) Uani 1 1 d . . .
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C27 C 0.5838(4) 0.9199(3) 0.2933(3) 0.0379(14) Uani 1 1 d . . .
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C28 C 0.4942(5) 0.9411(3) 0.3324(3) 0.0373(12) Uani 1 1 d . . .
H28 H 0.4886 0.9673 0.3836 0.045 Uiso 1 1 calc R . .
C29 C 0.4151(4) 0.9170(3) 0.2831(3) 0.0364(13) Uani 1 1 d . . .
H29 H 0.3463 0.9246 0.2943 0.044 Uiso 1 1 calc R . .
C30 C 0.6005(3) 0.7133(4) 0.4879(3) 0.0344(11) Uani 1 1 d . . .
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H32C H 0.6548 0.6601 0.6515 0.071 Uiso 1 1 calc R . .
C33 C 0.5860(4) 0.8252(3) 0.5706(3) 0.0363(13) Uani 1 1 d . . .
H33 H 0.5792 0.8584 0.6177 0.044 Uiso 1 1 calc R . .
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C36 C 0.3502(4) 0.8545(3) 0.4753(3) 0.0340(12) Uani 1 1 d . . .
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C38 C 0.3473(3) 0.7104(3) 0.4757(2) 0.0326(11) Uani 1 1 d . . .
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C39 C 0.3468(4) 0.7375(3) 0.5571(3) 0.0322(13) Uani 1 1 d . . .
C40 C 0.3407(4) 0.6828(3) 0.6299(3) 0.0467(15) Uani 1 1 d . . .
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H40B H 0.3746 0.6296 0.6191 0.070 Uiso 1 1 calc R . .
H40C H 0.2706 0.6720 0.6429 0.070 Uiso 1 1 calc R . .
C41 C 0.3477(4) 0.8260(3) 0.5554(3) 0.0339(13) Uani 1 1 d . . .
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C2 0.033(3) 0.026(3) 0.025(2) 0.004(2) 0.002(2) 0.008(2)
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C13 0.032(3) 0.0122(19) 0.026(2) 0.0041(17) 0.002(2) -0.005(2)
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C15 0.049(4) 0.029(3) 0.031(2) 0.005(2) 0.009(2) -0.003(2)
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C20 0.050(4) 0.041(3) 0.036(3) -0.007(2) 0.019(3) -0.001(3)
C21 0.061(5) 0.038(3) 0.023(2) -0.0048(19) 0.000(3) -0.009(3)
C22 0.040(3) 0.033(3) 0.025(3) -0.008(2) 0.002(2) -0.016(3)
C23 0.049(3) 0.024(2) 0.030(2) -0.0063(18) -0.003(3) -0.002(3)
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C35 0.031(3) 0.038(3) 0.037(2) 0.000(3) 0.012(2) 0.001(3)
C36 0.028(3) 0.034(3) 0.039(3) 0.005(2) 0.003(2) 0.001(3)
C37 0.033(3) 0.034(3) 0.030(2) 0.002(3) -0.010(2) -0.007(3)
C38 0.029(3) 0.034(3) 0.034(2) 0.001(2) -0.007(2) -0.009(3)
C39 0.025(3) 0.039(3) 0.033(3) 0.009(2) 0.001(2) -0.012(2)
C40 0.040(3) 0.060(4) 0.039(3) 0.016(2) 0.000(3) -0.017(3)
C41 0.028(3) 0.038(3) 0.035(3) -0.003(2) 0.004(2) -0.008(3)
B1 0.037(4) 0.019(3) 0.018(2) 0.002(2) 0.006(2) 0.002(3)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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F55A F -0.16172(11) 0.19179(10) 0.02137(7) 0.0489(3) Uani 1 1 d . . .
F56B F 0.28754(9) 0.79440(8) 0.61045(5) 0.0309(2) Uani 1 1 d . . .
F56A F 0.04264(11) 0.18186(10) 0.05881(7) 0.0482(3) Uani 1 1 d . . .
B1B B 0.37048(15) 0.74751(13) 0.47675(9) 0.0203(4) Uani 1 1 d . . .
B1A B 0.22818(16) 0.29381(14) 0.03654(9) 0.0217(4) Uani 1 1 d . . .
C1A C 0.40600(15) 0.11879(13) 0.30348(10) 0.0300(4) Uani 1 1 d . . .
H1AA H 0.4675 0.0882 0.3184 0.036 Uiso 1 1 calc R . .
C1B C 0.3749(2) 0.37044(19) 0.80924(11) 0.0468(6) Uani 1 1 d . . .
H1BA H 0.4106 0.4127 0.8529 0.056 Uiso 1 1 calc R . .
C2A C 0.32889(15) 0.16341(12) 0.34163(9) 0.0269(4) Uani 1 1 d . . .
H2AA H 0.3267 0.1699 0.3881 0.032 Uiso 1 1 calc R . .
C2B C 0.40075(17) 0.36733(17) 0.74871(11) 0.0380(5) Uani 1 1 d . . .
H2BA H 0.4580 0.4072 0.7421 0.046 Uiso 1 1 calc R . .
C3A C 0.26590(16) 0.20869(12) 0.30667(10) 0.0300(4) Uani 1 1 d . . .
H3AA H 0.2121 0.2533 0.3242 0.036 Uiso 1 1 calc R . .
C3B C 0.34390(19) 0.29127(16) 0.70022(11) 0.0393(5) Uani 1 1 d . . .
H3BA H 0.3544 0.2669 0.6533 0.047 Uiso 1 1 calc R . .
C4A C 0.30267(18) 0.19057(14) 0.24597(10) 0.0360(5) Uani 1 1 d . . .
H4AA H 0.2802 0.2212 0.2137 0.043 Uiso 1 1 calc R . .
C4B C 0.2808(2) 0.24722(17) 0.73051(15) 0.0542(7) Uani 1 1 d . . .
H4BA H 0.2404 0.1856 0.7090 0.065 Uiso 1 1 calc R . .
C5A C 0.39026(17) 0.13585(15) 0.24482(11) 0.0355(5) Uani 1 1 d . . .
H5AA H 0.4392 0.1202 0.2111 0.043 Uiso 1 1 calc R . .
C5B C 0.3015(2) 0.2966(2) 0.79836(14) 0.0577(8) Uani 1 1 d . . .
H5BA H 0.2769 0.2763 0.8329 0.069 Uiso 1 1 calc R . .
C6A C 0.24922(16) -0.10805(13) 0.15109(9) 0.0299(4) Uani 1 1 d . . .
H6AA H 0.2997 -0.1557 0.1537 0.036 Uiso 1 1 calc R . .
C6B C 0.06154(17) 0.44325(18) 0.81813(10) 0.0389(5) Uani 1 1 d . . .
H6BA H 0.0717 0.4864 0.8645 0.047 Uiso 1 1 calc R . .
C7A C 0.14083(16) -0.11011(13) 0.15948(9) 0.0283(4) Uani 1 1 d . . .
H7AA H 0.1019 -0.1594 0.1693 0.034 Uiso 1 1 calc R . .
C7B C 0.02839(15) 0.46770(17) 0.76256(10) 0.0358(5) Uani 1 1 d . . .
H7BA H 0.0113 0.5307 0.7633 0.043 Uiso 1 1 calc R . .
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C8A C 0.09413(16) -0.03961(14) 0.14213(9) 0.0298(4) Uani 1 1 d . . .
H8AA H 0.0163 -0.0302 0.1375 0.036 Uiso 1 1 calc R . .
C8B C 0.00967(16) 0.38613(16) 0.70790(10) 0.0357(5) Uani 1 1 d . . .
H8BA H -0.0240 0.3811 0.6632 0.043 Uiso 1 1 calc R . .
C9A C 0.17315(17) 0.00830(14) 0.12407(9) 0.0317(4) Uani 1 1 d . . .
H9AA H 0.1606 0.0561 0.1035 0.038 Uiso 1 1 calc R . .
C9B C 0.03233(18) 0.31133(17) 0.72900(11) 0.0412(5) Uani 1 1 d . . .
H9BA H 0.0157 0.2446 0.7019 0.049 Uiso 1 1 calc R . .
C10A C 0.26871(17) -0.03551(15) 0.12882(9) 0.0322(4) Uani 1 1 d . . .
H10A H 0.3355 -0.0229 0.1128 0.039 Uiso 1 1 calc R . .
C10B C 0.06295(18) 0.34742(18) 0.79775(11) 0.0421(5) Uani 1 1 d . . .
H10B H 0.0729 0.3104 0.8270 0.050 Uiso 1 1 calc R . .
C11A C 0.10033(14) 0.03110(11) 0.30266(8) 0.0220(3) Uani 1 1 d . . .
C11B C 0.22897(14) 0.47626(12) 0.67973(8) 0.0218(3) Uani 1 1 d . . .
C12B C 0.31430(15) 0.47076(12) 0.64092(8) 0.0238(3) Uani 1 1 d . . .
H12A H 0.3842 0.4448 0.6481 0.029 Uiso 1 1 calc R . .
C12A C 0.08422(15) 0.10181(12) 0.36351(8) 0.0258(4) Uani 1 1 d . . .
H12B H 0.1398 0.1505 0.3924 0.031 Uiso 1 1 calc R . .
C13B C 0.28317(16) 0.50639(12) 0.59043(9) 0.0263(4) Uani 1 1 d . . .
H13A H 0.3273 0.5105 0.5570 0.032 Uiso 1 1 calc R . .
C13A C -0.02158(16) 0.09373(13) 0.37541(9) 0.0295(4) Uani 1 1 d . . .
H13B H -0.0526 0.1343 0.4139 0.035 Uiso 1 1 calc R . .
C14A C -0.07604(16) 0.01798(13) 0.32286(9) 0.0286(4) Uani 1 1 d . . .
H14A H -0.1522 -0.0045 0.3177 0.034 Uiso 1 1 calc R . .
C14B C 0.17863(16) 0.53495(12) 0.59589(9) 0.0278(4) Uani 1 1 d . . .
H14B H 0.1357 0.5625 0.5669 0.033 Uiso 1 1 calc R . .
C15B C 0.14537(15) 0.51678(12) 0.64959(8) 0.0249(4) Uani 1 1 d . . .
H15A H 0.0738 0.5287 0.6639 0.030 Uiso 1 1 calc R . .
C15A C -0.00276(15) -0.02023(12) 0.27887(9) 0.0244(3) Uani 1 1 d . . .
H15B H -0.0201 -0.0739 0.2370 0.029 Uiso 1 1 calc R . .
C16B C 0.13037(16) 0.26059(12) 0.56237(10) 0.0298(4) Uani 1 1 d . . .
H16A H 0.1253 0.2307 0.5955 0.036 Uiso 1 1 calc R . .
C16A C 0.00008(18) 0.18460(16) 0.22439(11) 0.0387(5) Uani 1 1 d . . .
H16B H 0.0618 0.1820 0.2000 0.046 Uiso 1 1 calc R . .
C17B C 0.22065(16) 0.26601(13) 0.53209(10) 0.0331(4) Uani 1 1 d . . .
H17A H 0.2902 0.2396 0.5395 0.040 Uiso 1 1 calc R . .
C17A C -0.00810(17) 0.24811(14) 0.28780(12) 0.0361(5) Uani 1 1 d . . .
H17B H 0.0464 0.2985 0.3157 0.043 Uiso 1 1 calc R . .
C18B C 0.19488(17) 0.31496(14) 0.48901(9) 0.0340(5) Uani 1 1 d . . .
H18A H 0.2430 0.3285 0.4604 0.041 Uiso 1 1 calc R . .
C18A C -0.10752(17) 0.22793(14) 0.30410(11) 0.0348(4) Uani 1 1 d . . .
H18B H -0.1358 0.2620 0.3454 0.042 Uiso 1 1 calc R . .
C19B C 0.08853(17) 0.33983(14) 0.49265(9) 0.0315(4) Uani 1 1 d . . .
H19A H 0.0485 0.3743 0.4674 0.038 Uiso 1 1 calc R . .
C19A C -0.16065(17) 0.15176(14) 0.25146(11) 0.0364(5) Uani 1 1 d . . .
H19B H -0.2330 0.1229 0.2491 0.044 Uiso 1 1 calc R . .
C20B C 0.04877(15) 0.30637(13) 0.53817(9) 0.0298(4) Uani 1 1 d . . .
H20A H -0.0239 0.3142 0.5513 0.036 Uiso 1 1 calc R . .
C20A C -0.09402(18) 0.12473(16) 0.20236(11) 0.0396(5) Uani 1 1 d . . .
H20B H -0.1107 0.0729 0.1594 0.048 Uiso 1 1 calc R . .
C21A C 0.44441(16) -0.11813(14) 0.28826(10) 0.0313(4) Uani 1 1 d . . .
H21A H 0.4630 -0.1566 0.3146 0.047 Uiso 1 1 calc R . .
H21B H 0.4989 -0.0670 0.2999 0.047 Uiso 1 1 calc R . .
H21C H 0.4404 -0.1555 0.2419 0.047 Uiso 1 1 calc R . .
C21B C 0.3052(2) 0.58568(17) 0.91790(9) 0.0431(5) Uani 1 1 d . . .
H21D H 0.3325 0.6496 0.9425 0.065 Uiso 1 1 calc R . .
H21E H 0.3573 0.5437 0.9259 0.065 Uiso 1 1 calc R . .
H21F H 0.2381 0.5733 0.9320 0.065 Uiso 1 1 calc R . .
C22A C 0.33639(16) -0.01601(13) 0.39229(9) 0.0278(4) Uani 1 1 d . . .
H22A H 0.3684 -0.0583 0.4125 0.042 Uiso 1 1 calc R . .
H22B H 0.2679 0.0006 0.4074 0.042 Uiso 1 1 calc R . .
H22C H 0.3841 0.0398 0.4045 0.042 Uiso 1 1 calc R . .
C22B C 0.4092(2) 0.60669(18) 0.81635(11) 0.0494(7) Uani 1 1 d . . .
H22D H 0.4319 0.6681 0.8486 0.074 Uiso 1 1 calc R . .
H22E H 0.4015 0.6096 0.7724 0.074 Uiso 1 1 calc R . .
H22F H 0.4625 0.5634 0.8201 0.074 Uiso 1 1 calc R . .
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C23A C 0.23094(16) -0.17508(13) 0.29070(10) 0.0301(4) Uani 1 1 d . . .
H23A H 0.2669 -0.2124 0.3139 0.045 Uiso 1 1 calc R . .
H23B H 0.2165 -0.2112 0.2439 0.045 Uiso 1 1 calc R . .
H23C H 0.1637 -0.1572 0.3072 0.045 Uiso 1 1 calc R . .
C23B C 0.1986(2) 0.66025(16) 0.82803(12) 0.0546(7) Uani 1 1 d . . .
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H23E H 0.1281 0.6480 0.8382 0.082 Uiso 1 1 calc R . .
H23F H 0.1912 0.6637 0.7842 0.082 Uiso 1 1 calc R . .
C31B C 0.28366(13) 0.82751(11) 0.49013(8) 0.0194(3) Uani 1 1 d . . .
C31A C 0.29253(14) 0.23676(12) -0.02448(8) 0.0216(3) Uani 1 1 d . . .
C32B C 0.30763(15) 0.91327(12) 0.53967(8) 0.0242(3) Uani 1 1 d . . .
C32A C 0.24773(14) 0.17639(12) -0.08589(8) 0.0234(3) Uani 1 1 d . . .
C33B C 0.24777(16) 0.98870(12) 0.54741(9) 0.0278(4) Uani 1 1 d . . .
C33A C 0.30561(16) 0.12336(12) -0.13272(9) 0.0273(4) Uani 1 1 d . . .
C34B C 0.15789(15) 0.98241(12) 0.50319(9) 0.0259(4) Uani 1 1 d . . .
C34A C 0.41440(16) 0.12817(13) -0.11963(9) 0.0282(4) Uani 1 1 d . . .
C35B C 0.12929(14) 0.89970(12) 0.45330(8) 0.0219(3) Uani 1 1 d . . .
C35A C 0.46402(15) 0.18652(14) -0.05986(9) 0.0282(4) Uani 1 1 d . . .
C36B C 0.19122(13) 0.82567(11) 0.44834(8) 0.0183(3) Uani 1 1 d . . .
C36A C 0.40317(14) 0.23775(12) -0.01467(8) 0.0245(3) Uani 1 1 d . . .
C41B C 0.31863(13) 0.64989(11) 0.41971(8) 0.0202(3) Uani 1 1 d . . .
C41A C 0.26603(14) 0.40557(12) 0.06919(8) 0.0218(3) Uani 1 1 d . . .
C42B C 0.35171(15) 0.60733(13) 0.35947(9) 0.0249(4) Uani 1 1 d . . .
C42A C 0.33356(14) 0.45572(12) 0.04682(8) 0.0235(3) Uani 1 1 d . . .
C43B C 0.30857(17) 0.52313(13) 0.31443(9) 0.0291(4) Uani 1 1 d . . .
C43A C 0.36626(15) 0.54800(13) 0.07897(9) 0.0261(4) Uani 1 1 d . . .
C44B C 0.22671(17) 0.47754(12) 0.32796(9) 0.0312(4) Uani 1 1 d . . .
C44A C 0.32794(15) 0.59643(12) 0.13560(9) 0.0273(4) Uani 1 1 d . . .
C45B C 0.19002(15) 0.51578(12) 0.38686(9) 0.0270(4) Uani 1 1 d . . .
C45A C 0.25645(15) 0.55225(13) 0.15851(8) 0.0259(4) Uani 1 1 d . . .
C46B C 0.23630(14) 0.59918(12) 0.43055(8) 0.0212(3) Uani 1 1 d . . .
C46A C 0.22769(14) 0.45944(13) 0.12558(8) 0.0234(3) Uani 1 1 d . . .
C51B C 0.41026(13) 0.71693(12) 0.54053(8) 0.0206(3) Uani 1 1 d . . .
C51A C 0.09876(14) 0.28946(12) 0.01193(8) 0.0234(3) Uani 1 1 d . . .
C52B C 0.49130(14) 0.65699(12) 0.53630(8) 0.0225(3) Uani 1 1 d . . .
C52A C 0.05967(15) 0.34290(14) -0.02407(9) 0.0267(4) Uani 1 1 d . . .
C53B C 0.53223(14) 0.62619(12) 0.58532(9) 0.0248(3) Uani 1 1 d . . .
C53A C -0.04647(16) 0.34955(15) -0.04302(9) 0.0319(4) Uani 1 1 d . . .
C54B C 0.49157(14) 0.65409(12) 0.64334(9) 0.0240(3) Uani 1 1 d . . .
C54A C -0.12173(15) 0.29867(14) -0.02776(9) 0.0314(4) Uani 1 1 d . . .
C55B C 0.40966(14) 0.71135(12) 0.65010(8) 0.0233(3) Uani 1 1 d . . .
C55A C -0.08867(16) 0.24337(14) 0.00685(10) 0.0325(4) Uani 1 1 d . . .
C56B C 0.37032(14) 0.74040(12) 0.59950(8) 0.0222(3) Uani 1 1 d . . .
C56A C 0.01901(16) 0.23975(13) 0.02584(9) 0.0287(4) Uani 1 1 d . . .
C61B C 0.47313(15) 0.79442(14) 0.45817(10) 0.0292(4) Uani 1 1 d . . .
H61A H 0.4994 0.8519 0.4940 0.044 Uiso 1 1 calc R . .
H61B H 0.4515 0.8077 0.4182 0.044 Uiso 1 1 calc R . .
H61C H 0.5298 0.7516 0.4511 0.044 Uiso 1 1 calc R . .
C61A C 0.25691(16) 0.24771(14) 0.09270(9) 0.0291(4) Uani 1 1 d . . .
H61D H 0.2350 0.1816 0.0744 0.044 Uiso 1 1 calc R . .
H61E H 0.2191 0.2776 0.1297 0.044 Uiso 1 1 calc R . .
H61F H 0.3338 0.2564 0.1076 0.044 Uiso 1 1 calc R . .
Br1 Br 0.38888(13) 0.90320(6) 0.90121(5) 0.0976(4) Uani 0.50 1 d P . .
C101 C 0.4839(6) 0.9793(4) 0.9778(3) 0.0556(15) Uani 0.50 1 d P . .
C102 C 0.571(2) 0.9528(15) 0.9701(12) 0.129(8) Uani 0.50 1 d P . .
C103 C 0.6572(6) 1.0172(8) 1.0315(6) 0.078(3) Uani 0.50 1 d P . .
C105 C 0.5691(12) 0.9586(8) 0.9793(6) 0.047(2) Uani 0.50 1 d P . .
C104 C 0.3545(4) 0.9270(5) 0.9311(3) 0.0362(11) Uani 0.50 1 d P . .
C106 C 0.4776(7) 0.8983(4) 0.9157(3) 0.0509(14) Uani 0.50 1 d P . .

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F33B 0.0536(8) 0.0229(6) 0.0348(6) -0.0039(5) 0.0026(6) -0.0017(5)
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F35A 0.0202(6) 0.0527(8) 0.0473(7) 0.0075(6) 0.0084(5) 0.0070(5)
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C2A 0.0286(10) 0.0215(8) 0.0262(8) 0.0065(7) -0.0050(7) -0.0089(7)
C2B 0.0264(10) 0.0526(13) 0.0383(11) 0.0186(10) 0.0061(8) 0.0180(9)
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C3B 0.0441(13) 0.0418(12) 0.0348(11) 0.0132(9) 0.0127(9) 0.0236(10)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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H17B H 0.5800 -0.0503 0.2099 0.080 Uiso 1 1 calc R . .
H17C H 0.5478 -0.0470 0.1088 0.080 Uiso 1 1 calc R . .
C3 C 0.3829(3) 0.20576(9) 0.35410(15) 0.0405(6) Uani 1 1 d . . .
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H7A H 0.7586 -0.0258 0.3139 0.117 Uiso 1 1 calc R . .
H7B H 0.6468 -0.0396 0.3650 0.117 Uiso 1 1 calc R . .
H7C H 0.8039 -0.0229 0.4155 0.117 Uiso 1 1 calc R . .
C27 C 0.5870(2) 0.23871(7) 0.15322(14) 0.0272(4) Uani 1 1 d . . .
H27 H 0.5963 0.2643 0.1958 0.033 Uiso 1 1 calc R . .
H23 H 0.649(4) 0.1778(14) 0.216(3) 0.105(14) Uiso 1 1 d . . .

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C22 0.0209(10) 0.0276(11) 0.0407(12) -0.0043(9) 0.0121(9) 0.0052(8)
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C20 0.0252(11) 0.0357(12) 0.0339(12) -0.0060(9) -0.0055(9) 0.0055(9)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Fe1 C21 2.072(2) . ?
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C34 C33 C32 119.16(19) . . ?
F9 C43 C44 119.67(19) . . ?
F9 C43 C42 120.85(19) . . ?
C44 C43 C42 119.47(19) . . ?
F14 C37 C38 120.0(2) . . ?
F14 C37 C36 120.2(2) . . ?
C38 C37 C36 119.8(2) . . ?
F1 C30 C31 114.43(18) . . ?
F1 C30 C29 121.15(18) . . ?
C31 C30 C29 124.42(19) . . ?
F8 C44 C45 120.9(2) . . ?
F8 C44 C43 120.6(2) . . ?
C45 C44 C43 118.45(19) . . ?
F3 C32 C31 120.6(2) . . ?
F3 C32 C33 120.60(19) . . ?
C31 C32 C33 118.76(18) . . ?
F13 C38 C37 120.4(2) . . ?
F13 C38 C39 120.6(3) . . ?
C37 C38 C39 118.9(2) . . ?
F10 C42 C43 115.28(17) . . ?
F10 C42 C41 119.64(17) . . ?
C43 C42 C41 125.08(19) . . ?
F11 C40 C39 114.9(2) . . ?
F11 C40 C35 120.68(18) . . ?
C39 C40 C35 124.4(2) . . ?
F7 C45 C44 119.61(19) . . ?
F7 C45 C46 120.42(19) . . ?
C44 C45 C46 119.95(19) . . ?
F12 C39 C38 120.0(2) . . ?
F12 C39 C40 120.2(2) . . ?
C38 C39 C40 119.8(2) . . ?
C26 C27 C23 107.80(19) . . ?
C26 C27 Fe1 70.77(12) . . ?
C23 C27 Fe1 67.31(11) . . ?

_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              27.47
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    0.350
_refine_diff_density_min   -0.300
_refine_diff_density_rms    0.052
#===end
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